

=> fil reg
FILE 'REGISTRY' ENTERED AT 10:45:09 ON 16 SEP 2002
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Structure 5b

STRUCTURE FILE UPDATES: 15 SEP 2002 HIGHEST RN 451445-11-7
DICTIONARY FILE UPDATES: 15 SEP 2002 HIGHEST RN 451445-11-7

TSCA INFORMATION NOW CURRENT THROUGH MAY 20, 2002

Please note that search-term pricing does apply when
conducting SmartSELECT searches.

Crossover limits have been increased. See HELP CROSSOVER for details.

Experimental and calculated property data are now available. See HELP PROPERTIES for more information. See STNote 27, Searching Properties in the CAS Registry File, for complete details:
<http://www.cas.org/ONLINE/STN/STNOTES/stnotes27.pdf>

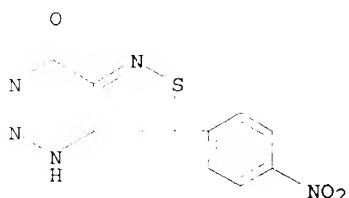
=> d que 11;d que 12
L1 44 SEA FILE=REGISTRY ABB=ON PLU=ON NSC3-N3C3/ES

L2 4 SEA FILE=REGISTRY ABB=ON PLU=ON 333.1144/RID

=> d 12 ide can 1-4

L2 ANSWER 1 OF 4 REGISTRY COPYRIGHT 2002 ACS
RN 72633-09-1 REGISTRY
CN Isothiazolo[4,3-d]-1,2,3-triazin-4(1H)-one, 7-(4-nitrophenyl)- (9CI) (CA
INDEX NAME)
FS 3D CONCORD
MF C10 H5 N5 O3 S
LC STN Files: BEILSTEIN*, CA, CAPLUS, CASREACT
(*File contains numerically searchable property data)

*↳ more matches
clumped structures*



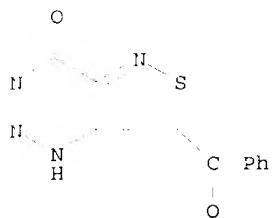
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1967 TO DATE)
1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 92:76382

L2 ANSWER 2 OF 4 REGISTRY COPYRIGHT 2002 ACS

RN 72632-96-3 REGISTRY
 CN Isothiazolo[4,3-d]-1,2,3-triazin-4(1H)-one, 7-benzoyl- (9CI) (CA INDEX NAME)
 FS 3D CONCORD
 MF C11 H6 N4 O2 S
 LC STN Files: BEILSTEIN*, CA, CAPLUS, CASREACT
 (*File contains numerically searchable property data)

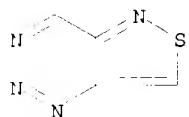


PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1967 TO DATE)
 1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

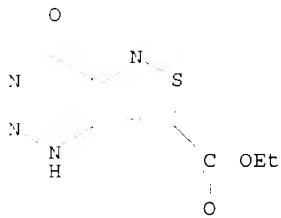
REFERENCE 1: 92:76382

L2 ANSWER 3 OF 4 REGISTRY COPYRIGHT 2002 ACS
 RN 55402-82-9 REGISTRY
 CN Isothiazolo[4,3-d]-1,2,3-triazine (9CI) (CA INDEX NAME)
 FS 3D CONCORD
 MF C4 H2 N4 S
 CI RPS



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L2 ANSWER 4 OF 4 REGISTRY COPYRIGHT 2002 ACS
 RN 54968-80-8 REGISTRY
 CN Isothiazolo[4,3-d]-1,2,3-triazine-7-carboxylic acid, 1,4-dihydro-4-oxo-, ethyl ester (9CI) (CA INDEX NAME)
 FS 3D CONCORD
 MF C7 H6 N4 O3 S
 LC STN Files: BEILSTEIN*, CA, CAPLUS, CASREACT
 (*File contains numerically searchable property data)



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

2 REFERENCES IN FILE CA (1967 TO DATE)
2 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 92:76382

REFERENCE 2: 82:139991

=> fil hcaplus
FILE 'HCAPLUS' ENTERED AT 10:47:16 ON 16 SEP 2002
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FILE COVERS 1907 - 16 Sep 2002 VOL 137 ISS 12
FILE LAST UPDATED: 15 Sep 2002 (20020915/ED)

This file contains CAS Registry Numbers for easy and accurate substance identification.

CAS roles have been modified effective December 16, 2001. Please check your SDI profiles to see if they need to be revised. For information on CAS roles, enter HELP ROLES at an arrow prompt or use the CAS Roles thesaurus (/RL field) in this file.
'OBI' IS DEFAULT SEARCH FIELD FOR 'HCAPLUS' FILE

=> s 12

L3 2 L2

=> d .ca 1-2

L3 ANSWER 1 OF 2 HCAPLUS COPYRIGHT 2002 ACS
ACCESSION NUMBER: 1980:76382 HCAPLUS

DOCUMENT NUMBER: 92:76382
 TITLE Synthesis and reactions of 4-aminoisothiazoles
 AUTHOR(S): Gewald, Karl; Bellmann, Peter
 CORPORATE SOURCE: Sekt. Chem., Tech. Univ. Dresden, Dresden, DDR-8027,
 Ger. Dem. Rep.
 SOURCE Liebigs Ann. Chem. (1979), (10), 1534-46
 CODEN: LACHDL
 DOCUMENT TYPE: Journal
 LANGUAGE: German
 AB 4-MeC₆H₄ON:CRCN (R = CONH₂, CO₂Et, COPh, Ph, 4-O₂NC₆H₄) reacted with F:CH₂SH (R₁ = COPh, CO₂Et, COMe, CO₂H, C₆H₄NO₂-4, CHO, Ph) to give the corresponding aminoisothiazoles I via the intermediates R₁CH₂SN:CRCN. Decarboxylation gave 5-unsubstituted 4-aminoisothiazoles, e.g., reaction of I (R = CONH₂, R₁ = CO₂Et) with HCl gave 3-carboxy-4-aminoisothiazole, which was heated with Ac₂O to give 4-acetamidoisothiazole. I were also converted into the ring systems II (R₁ = COPh, CO₂Et, C₆H₄NO₂-4), III (R₁ = CO₂Et, COMe), IV (R = CONH₂, Ph, C₆H₄NO₂-4), and V (R = CONH₂, CO₂Et; R₂ = H, Me).
 CC 28-7 (Heterocyclic Compounds (More Than One Hetero Atom))
 IT 54968-79-5P 54968-80-8P 72632-83-8P 72632-86-1P
 72632-88-3P 72632-91-8P 72632-92-9P 72632-93-0P 72632-94-1P
 72632-95-2P 72632-96-3P 72632-97-4P 72632-98-5P
 72632-99-6P 72633-00-2P 72633-01-3P 72633-02-4P 72633-03-5P
 72633-04-6P 72633-05-7P 72633-06-8P 72633-08-0P 72633-09-1P
 FL: SPN (Synthetic preparation); PREP (Preparation)
 (prepn. of)

L3 ANSWER 2 OF 2 HCPLUS COPYRIGHT 2002 ACS
 ACCESSION NUMBER: 1975:139991 HCPLUS
 DOCUMENT NUMBER: 82:139991
 TITLE New synthesis of 4-aminoisothiazoles
 AUTHOR(S): Gewald, Karl; Bellmann, Peter; Jaensch, Hans J.
 CORPORATE SOURCE: Sekt. Chem., Tech. Univ. Dresden, Dresden, E. Ger.
 SOURCE Z. Chem. (1975), 15(1), 18-19
 CODEN: ZECRAL
 DOCUMENT TYPE: Journal
 LANGUAGE: German
 AB Aminoisothiazoles I (R = CONH₂, CO₂Et; R₁ = CO₂Et, Ac) were prep'd. in 48-60% yield by treating NCCR:NO₃SC₆H₄Me-p with R₁CH₂SH in the presence of base at <40.degree.. H₂NCO(CN):NSCH₂CO₂Et was also isolated and diazotized, giving the isothiazolotriazinone II (X = N). Condensation of I (R = CONH₂, R₁ = CO₂Et) with HC(OEt)₃ gave II (X = CH).
 CC 28-7 (Heterocyclic Compounds (More Than One Hetero Atom))
 IT 54968-75-1P 54968-76-2P 54968-79-5P 54968-80-8P
 FL: SPN (Synthetic preparation); PREP (Preparation)
 (prepn. of)